TITLE KINETICS OF SLURRY PHASE FISCHER-TROPSCH SYNTHESIS

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ABSTRACT

OBJECTIVES

The overall objective of this project is to develop a comprehensive kinetic model for slurry phase Fischer-Tropsch synthesis on iron catalysts. This model will be validated with experimental data obtained in a stirred tank slurry reactor (STSR) over a wide range of process conditions. This model will be able to predict concentrations of all reactants and major product species (H_2O, CO_2, linear 1- and 2-olefins, and linear paraffins) as a function of reaction conditions in the STSR. Kinetic model will be useful for preliminary reactor design and process economics study.

METHODOLOGY

After a thorough review of literature kinetic models will be formulated utilizing the current state-of-the-art understanding of reaction mechanisms for formation of reaction intermediates and hydrocarbon products. Models will be based on adsorption/desorption phenomena for reactants and product species. The importance of secondary 1-olefin readsorption reaction, and of chain length dependent solubilities, adsorptivities and/or diffusivities will be critically examined and incorporated if necessary. Models will be continually updated on the basis of experimental data obtained in the STSR, and subsequent data analysis. Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach and the concept of rate limiting step result in a large number of competing kinetic models. Discrimination between the rival models will

be based upon the goodness of fit, supplemented with statistical tests on parameter values and the physicochemical meaningfulness of the estimated parameter values.

Experiments will be conducted in a 1 dm^3 STSR (Autoclave Engineers). Experimental conditions will be chosen to eliminate gas-liquid mass transfer resistance, catalyst settling and intraparticle diffusional limitations. Synthesis gas feed H_2/CO molar ratio will vary from 0.67 (coal derived syngas) to 2 (natural gas derived syngas). Reaction temperature will be in the range between 230 and 260°C, and reaction pressure between 1.0 and 2.5 MPa. For a given set of T, P and feed composition, the gas flow rate (i.e. gas space velocity) will be varied to obtain data at different levels of conversion. Baseline conditions will be repeated periodically to assess the extent of catalyst deactivation.

ACCOMPLISHMENTS

Mr. Jian Wang (Ph. D. student) joined the project in January 2003. He is becoming familiar with operation of the slurry reactor and auxiliary instruments, product analysis by gas chromatography, and use of existing software for product identification and mass balance calculations.

PLANS FOR THE NEXT YEAR

- Synthesis of precipitated iron F-T catalyst;
- Kinetic experiments in the stirred tank slurry reactor;
- Literature review and development of kinetic models.

Articles and Presentations

None.

Students and post-doctoral fellows supported under this grant

Mr. Jian Wang (Ph. D. Student)

Dr. Wen-Ping Ma (post-doctoral fellow)

TITLE IMPROVED IRON CATALYSTS FOR SLURRY PHASE FISCHER-TROPSCH SYNTHESIS

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ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Bukur, D. B. and Sivaraj, C., "Supported Iron Catalysts for Slurry Phase Fischer-Tropsch Synthesis", Applied Catalysis A, 231, 201-214 (2002).

Pham, H. N., Nowicki, L., Xu, J., Datye, A. K., Bukur, D. B. and Bartholomew, C., "Attrition Resistance of Supports for Iron Fischer-Tropsch Catalysts", submitted to I&ECR.

Conference Presentations

Dragomir B. Bukur, Ketil F. Hanssen and Chokkaram Sivaraj, "Supported Iron Catalysts for Fischer-Tropsch Synthesis", paper presented at the AICHE Spring National meeting, April 2001, Houston, Texas.

Dragomir B. Bukur, Wen-Ping Ma, Victor H. Carreto Vazquez, Lech Nowicki and Adeyinka A. Adeyiga, " Spray Dried Iron Catalysts for Slurry Phase Fischer-Tropsch Synthesis", paper to be presented at the 226th ACS National meeting, September, 2003, New York City, New York.

Dragomir B. Bukur, Lech Nowicki, Abhaya K. Datye and Hien N. Pham, "Attrition Resistant Iron Catalysts for Synthesis Gas Conversion to Liquid Fuels", paper to be presented at the AICHE National meeting, November 2003, San Francisco, California.

Students and post-doctoral fellows supported under this grant

Mr. Victor Carreto-Vazquez (M. Sc. Student) – Contributions: catalyst synthesis and spray drying, characterization by SEM, and PSD measurements.

Mr. Jian Wang (Ph. D. Student) –catalyst testing in a STSR.

Dr. Wen-Ping Ma (post-doctoral fellow) has been primarily responsible for catalyst testing in slurry reactors.